

Accelerating the estimation of 3D spatially resolved T_2 distributions

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Abstract

Obtaining quantitative, 3D spatially-resolved T_2 distributions (T_2 maps) from magnetic resonance data is of importance in both medical and porous media applications. Due to the long acquisition time, there is considerable interest in accelerating the experiments by applying undersampling schemes during the acquisition and developing reconstruction techniques for obtaining the 3D T_2 maps from the undersampled data. A multi-echo spin echo pulse sequence is used in this work to acquire the undersampled data according to two different sampling patterns: a conventional coherent sampling pattern where the same set of lines in k -space is sampled for all equally-spaced echoes in the echo train, and a proposed incoherent sampling pattern where an independent set of k -space lines is sampled for each echo. The conventional reconstruction technique of total variation regularization is compared to the more recent techniques of nuclear norm regularization and Nuclear Total Generalized Variation (NTGV) regularization. It is shown that best reconstructions are obtained when the data acquired using an incoherent sampling scheme are processed using NTGV regularization. Using an incoherent sampling pattern and NTGV regularization as the reconstruction technique, quantitative results are obtained at sampling percentages as low as 3.1% of k -space, corresponding to a 32-fold decrease in the acquisition time, compared to a fully sampled dataset.

Keywords: 3D T_2 map, compressed sensing, multi-echo spin echo, sampling pattern.

1.Introduction

Nuclear Magnetic Resonance (NMR) relaxation time constant distributions provide information and insights in many areas of application. In medicine, changes in the distribution of the spin-spin relaxation time constant, T_2 , are used to indicate tissue pathologies [1, 2]. Spatially-resolved T_2 distributions, which will be referred to as T_2 maps, have enabled the spatial localization of pathologies [3, 4]. In the study of porous media, T_2 distributions are used in pore size distribution and structure elucidation [5, 6] and in fluid characterisation [7, 8]. T_2 maps have enabled the determination of the local pore structure, pore saturation and wettability [9-15].

The principle of obtaining a T_2 map of dimension d ($d = 1, 2$ or 3 for a 1D, 2D or 3D T_2 map) is similar across the plethora of different experimental techniques. A series of p T_2 weighted images of dimension d is acquired, and the T_2 distribution is extracted pixel-wise using a numerical solution to a Fredholm integral of the first kind, also known as an Inverse Laplace Transform (ILT) algorithm, or some other single or multi-exponential fitting method. The experimental techniques differ in the way the T_2 weighted images are acquired. They can be categorized into experimental techniques which use either a variable echo time or keep the echo time fixed and vary the number of echoes in the echo train. The most widely used technique with a variable echo time is the Single Echo Spin Echo (SESE) pulse sequence [16, 17]. Although the SESE sequence is very robust, the acquisition time is prohibitively long. A single line of k -space is read out at each echo and a single echo is formed for each excitation. Therefore, the acquisition time scales approximately linearly with $n^{d-1}p$, with n being the number of points in each k -space dimension (assuming isotropic sampling). The most commonly used experimental technique with a fixed echo time is the Multi-Echo Spin Echo (MESE) pulse sequence [18-21]. A single line of k -space is sampled at each echo, but multiple echoes (an echo train) are formed for each excitation. Therefore, the acquisition time scales approximately linearly with n^{d-1} , which is a significant improvement over the acquisition time of the SESE method. The MESE pulse sequence is often referred to by different names depending on the application. For example, when used to obtaining T_2 contrast images, it is referred to as a Rapid Acquisition with Relaxation Enhancement (RARE) pulse sequence [22, 23]. The main disadvantage of the MESE technique is the

use of a train of slice-selective refocusing pulses, which, if not perfect, can lead to complex stimulated echo patterns [24, 25]. Another technique with a fixed echo time is the Spin Echo - Single Point Imaging (SE-SPI) pulse sequence [26-30]. The SE-SPI pulse sequence forms a train of p spin echoes for each excitation and at each echo a single point in k -space is sampled. As a result, the acquisition time scales approximately linearly with n^d , which is significantly longer than the acquisition time with an MESE pulse sequence. However, its main advantage is the capability to use much shorter echo times. This has enhanced the capability of magnetic resonance to study fluids characterized by sub-millisecond T_2 relaxation time constants in porous media.

This manuscript is concerned with obtaining 3D T_2 maps, which in application to porous media, would open opportunities for characterising the local pore structure, pore saturation and wettability. The major problem associated with obtaining 3D T_2 maps is the long acquisition time; for example, the acquisition time for a fully sampled dataset sampled with an SE-SPI technique is in the order of days [29]. The system under investigation may not be stable during such a long acquisition time, or one might wish to study a system that is evolving with time. Thus, there is a strong motivation to reduce the data acquisition time, whilst retaining the quantitative nature of the measurement. Without undersampling, the MESE technique offers the shortest acquisition time compared to the SESE and SE-SPI techniques, as discussed above. However, in most cases, this is still prohibitively long; for the system under consideration in this manuscript, acquiring a fully sampled data set with an MESE technique takes ~ 16 h. The focus of this work is in exploring undersampling schemes and reconstruction techniques for obtaining 3D T_2 maps from data acquired using an MESE technique. Compressed Sensing (CS) methods [31, 32] have recently become of increasing interest in reducing MRI acquisition times. The main principle of CS is that it is possible, with a high probability, to reconstruct a signal from far fewer samples than is required by the classical sampling theory [33, 34], provided the sampling is done randomly and the signal is sparse in some domain. Using CS, it has become possible, for example, to rapidly image single-phase [35, 36] and multi-phase [37] displacement processes in rock core floods using 3D MRI.

In this work, an experimental implementation of an MESE pulse sequence to acquire a 3D T_2 map from undersampled MRI data is demonstrated. A conventional sampling pattern where the same set of lines in k -space is sampled for all equally-spaced echoes in

the echo train (a coherent sampling pattern) is compared to a proposed sampling pattern where an independent set of k -space lines is sampled for each echo (an incoherent sampling pattern). Further, the performance of the conventional reconstruction technique of total variation regularization [38, 39] is compared with the performance of the more recent reconstruction techniques of nuclear norm regularization [40] and nuclear total generalized variation regularization [41, 42]. It is shown that using an incoherent sampling pattern and nuclear total generalized variation regularization as the reconstruction technique, quantitative 3D T_2 maps are obtained even at sampling percentages of 3.1% of k -space, corresponding to a 32-fold decrease in the acquisition time.

The paper is structured as follows. The experimental technique and materials used are described in Section 2. Section 3 introduces the different reconstruction methods and describes the algorithms used in the reconstruction process. The results and discussion are presented in Section 4.

2. Materials and methods

The acquisition of a 3D spatially resolved T_2 map was performed on the sample illustrated in Fig. 1(a). The sample was composed of 7 tubes of 10 mm diameter, bound in a circular arrangement. Each tube was filled up to a height of 40 mm; in the bottom 20 mm by a gadolinium chloride ($\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$) solution and in the top 20 mm by polydimethylsiloxane, trimethylsiloxo terminated (Alfa Aesar), which will be referred to as PDMS oil. Gadolinium chloride solutions of three different concentrations were used: 0.82 mM (fluid A), 0.55 mM (fluid B) and 0.22 mM (fluid C). The allocation of the gadolinium chloride solutions to particular tubes is shown in Fig. 1(a). PDMS oils of three different molecular weights were used: 28 kDa (fluid D), 9 kDa (fluid E) and 2 kDa (fluid F). Again, the allocation of the PDMS oils to particular tubes is given in Fig. 1(a).

All magnetic resonance experiments were conducted on a Bruker vertical superwide bore superconducting magnet with a static magnetic field strength of 7.1 T (^1H Larmor frequency 300.88 MHz for ^1H) coupled to a Bruker Avance III spectrometer. A radio-frequency (r.f.) coil of diameter 66 mm was used and the maximum magnetic field gradient strength available was 77 G cm^{-1} .

The T_2 distributions for each individual fluid used, obtained using a single shot CPMG experiment with echo time 15 ms and processed using L_1 regularization, are shown in Fig. 1(b). L_1 regularization was selected based on the fact that the PDMS oils D and E did not show mono-exponential behaviour in the T_2 decay and the conventional Tikhonov regularization method was unable to distinguish the two peaks of fluid D in the T_2 distribution [43]. The T_2 distribution for each individual fluid was unchanged before and after the experiment, indicating that the gadolinium chloride remained largely dissolved only in the water solution and did not affect the T_2 distribution of the PDMS oil.

The MESE pulse sequence used hard pulses of duration 82.5 μs and 165 μs for 90° and 180° r.f. excitations, respectively. The pulse sequence was designed for 3D imaging with a field-of-view of 35 mm \times 35 mm \times 45 mm, and respective spatial resolution of 547 μm \times 547 μm \times 703 μm , with the first two dimensions being phase-encoded directions (k_{p1} and k_{p2}) and the third dimension being the read direction, k_r (which was parallel to the longitudinal axis of the bundle of tubes). A dwell time of 5 μs , echo time of 15 ms and repetition time of 3.5 s were used. Each echo train was composed of 64 echoes.

Undersampling was performed on the two phase directions of k -space and sampling percentages of 100% (fully sampled), 50%, 25%, 12.5%, 6.3% and 3.1% were investigated, with corresponding acquisition times of 16 h, 8 h, 4 h, 2 h, 1 h and 30 min. For the two undersampled dimensions, the 2D sampling pattern followed a bi-level approach [44]. The central 3 \times 3 out of the 64 \times 64 pixels of k -space were fully sampled, while the location of subsequent points was chosen at random, with the density of points following a Gaussian distribution from the centre of k -space with a standard deviation of 15% of the largest k -space value. With these two undersampled dimensions (k_{p1} and k_{p2}) and a fully sampled third dimension (k_r), the Sidelobe-to-Peak Ratio (SPR) [38] of the density-compensated point-spread function of the 3D sampling pattern was 0, 0.029, 0.059, 0.091, 0.141 and 0.246 for the corresponding sampling percentages of 100%, 50%, 25%, 12.5%, 6.3% and 3.1% of k -space. Two sampling patterns, illustrated in Fig. 2, were investigated: a conventional coherent sampling pattern where the same set of lines in k -space is sampled in the read direction for all echoes in the echo train, and a proposed incoherent sampling pattern where a different set of k -space line is sampled in the read direction for each echo. Once the sampling percentage and pattern was selected,

the choice of the specific k -space lines to be read out in each successive echo within each echo train was randomised. An optimal set of randomised trajectories was selected such that the gradient dissipation was distributed homogenously between the different echo trains, so that the impact of the diffusive attenuation of the signal due to the gradients applied during the echo train was kept to a minimum.

3.Reconstruction techniques

Obtaining the 3D spatially resolved T_2 map from undersampled MRI data consists of two steps. The first step is the reconstruction of p T_2 -weighted images of size $n \times n \times n$, from the undersampled data. In the second step, the T_2 -weighted images serve as an input to an ILT algorithm, or a single or multi-exponential fitting procedure to obtain the T_2 distribution in each pixel. This work focuses on the first step. Three different reconstruction techniques are compared with the case of Zero-Filling (ZF). The reconstruction techniques used are: Total Variation (TV), Nuclear Norm (NN) and Nuclear Total Generalized Variation (NTGV) regularization. The reconstruction techniques are outlined below. The following definitions are used in the outline of the reconstruction techniques. \underline{U} is the desired $n \times n \times n \times p$ matrix containing the p T_2 -weighted images. $\hat{\underline{U}}$ is the $n^3 \times p$ matrix constructed by stacking the columns of each individual image of \underline{U} in a larger column. \underline{u} is the $n^3 p \times 1$ vector constructed by stacking the columns of $\hat{\underline{U}}$ in a larger column. Let \underline{f} be an $n^3 \times n^3$ Fourier matrix which, when applied on an $n^3 \times 1$ vector \underline{x} which is constructed by stacking the columns of an $n \times n \times n$ matrix \underline{X} in a larger column, performs the 3D Fourier transform of \underline{X} and stacks the columns of the resulting matrix in a larger column. The $n^3 p \times n^3 p$ matrix \underline{F} is defined as $\underline{F} = \underline{I}_p \otimes \underline{f}$, where \underline{I}_p is the identity matrix of size $p \times p$ and \otimes denotes the Kronecker product. When \underline{F} is applied to \underline{u} , the 3D Fourier transform of each individual T_2 -weighted image is performed and the results are stored in an $n^3 p \times 1$ matrix. The $m \times n^3 p$ undersampling matrix \underline{S} ($m \ll n^3 p$) is defined such that, when applied to an $n^3 p \times 1$ vector, picks only m of its entries.

With these definitions, the undersampled $m \times 1$ signal, \underline{y} , acquired from an MESE experiment can be expressed as:

$$\underline{y} = \underline{S} \underline{F} \underline{u} + \underline{e} , \quad (1)$$

where \underline{e} is an inherent noise vector of size $m \times 1$. The simplest reconstruction technique is commonly referred to as Zero-Filling (ZF), which consists of estimating \underline{u} from:

$$\underline{u} = \underline{F}^{-1} \underline{S}^T \underline{y}. \quad (2)$$

ZF reconstructions are typically sub-optimal because they are dominated by noise and undersampling artefacts. Better reconstructions can be obtained by incorporating some prior information about \underline{u} in the reconstruction process, by performing what is referred to as regularization. The most common prior information utilised for images is the fact that they are sparse in a TV domain [45]. TV regularization consists of estimating \underline{u} from:

$$\underline{u} = \arg \min_{\underline{u}} \left(\frac{1}{2} \left\| \underline{S} \underline{F} \underline{u} - \underline{y} \right\|_2^2 + \alpha \left\| \underline{R} \underline{u} \right\|_{2,1} \right). \quad (3)$$

\underline{R} is a $3n^3p \times n^3p$ matrix which performs the first derivative of each individual 3D T_2 -weighted image in all three spatial dimensions, with Neumann boundary conditions. $\left\| \underline{R} \underline{u} \right\|_{2,1}$ is defined as in the work of Benning *et al.* [46]. The regularization parameter, α , controls the amount of regularization imposed. The application of TV regularization is based on the observation that most images have large regions of constant intensity.

Other prior information that can be used in improving reconstructions is the fact that the pixel-wise magnitude decays between different T_2 -weighted images are highly correlated [47-51]. This is mathematically translated into $\hat{\underline{U}}$ having a low rank. It is a well-known result in linear algebra that the number of non-zero singular values of $\hat{\underline{U}}$ is equal to the rank of $\hat{\underline{U}}$. Therefore, it is in theory possible to improve the reconstructions by constraining $\hat{\underline{U}}$ to have a minimal number of non-zero singular values. In practice, this is computationally intractable, and the problem is relaxed by constraining $\hat{\underline{U}}$ to have a minimal sum of singular values; the sum of singular values is referred to as the nuclear norm, $\left\| \hat{\underline{U}} \right\|_*$. Nuclear Norm (NN) regularization consists of estimating \underline{u} from:

$$\underline{u} = \arg \min_{\underline{u}} \left(\frac{1}{2} \left\| \underline{S} \underline{F} \underline{u} - \underline{y} \right\|_2^2 + \alpha \left\| \hat{\underline{U}} \right\|_* \right). \quad (4)$$

The regularization parameter, α , controls the amount of regularization imposed.

In summary, TV regularization uses prior information about the individual T_2 -weighted images to improve the reconstructions, while NN regularization uses the relationship between the different T_2 -weighted images to improve the reconstructions. The natural extension is to combine these regularization techniques such that the reconstructions

inherit the best features from TV and NN regularization. One such technique is Nuclear Total Generalized Variation (NTGV) which consists of estimating \underline{u} from:

$$\underline{u} = \arg \min_{\underline{u}, \underline{w}} \left(\frac{1}{2} \left\| \underline{S} \underline{F} \underline{u} - \underline{y} \right\|_2^2 + \alpha \left\| \underline{\hat{U}} - \underline{\hat{W}} \right\|_* + \beta \left\| \underline{R} \underline{w} \right\|_{2,1} \right). \quad (5)$$

$\underline{\hat{W}}$ is an auxiliary $n^3 \times p$ matrix and \underline{w} is the $n^3 p \times 1$ vector constructed by stacking the columns of $\underline{\hat{W}}$ in a larger column. The second term enforces the reconstruction to inherit good features from NN regularization while the third term enforces the reconstruction to inherit good features from TV regularization. The regularization parameters, α and β , control the amount of regularization imposed. NTGV regularization is an extension of Total Generalized Variation (TGV) [52], which has been used in CS MRI to retain both sharp edges and smooth features in reconstructions [46, 53-55]. NTGV regularization has been previously used in processing the data obtained from a joint MR-PET scanner [41, 42], but has not been used in obtaining T_2 maps.

It is possible to write TV, NN and NTGV regularization as similar minimization problems, such that the same algorithm, the Primal-Dual Hybrid Gradient Method (PDHGM) [56] can be used to numerically solve them. This is discussed in the appendix, where pseudocodes and practical guidance for the numerical solution of all three regularization methods are given.

The reconstructed T_2 -weighted images obtained from the different reconstruction techniques were compared using the peak-signal-to-noise ratio (PSNR) metric:

$$\text{PSNR} = 20 \log_{10} \left(\frac{n^3 p \max(\underline{u}_{\text{FS}})}{\left\| \underline{u} - \underline{u}_{\text{FS}} \right\|_2^2} \right). \quad (6)$$

\underline{u} refers to the T_2 -weighted images obtained from undersampled MRI data processed using either zero-filling, TV regularization, NN regularization or NTGV regularization. $\underline{u}_{\text{FS}}$ refers to the T_2 -weighted images obtained from a fully sampled experiment. The reconstruction with the larger PSNR is the better reconstruction. The perfect reconstruction has $\text{PSNR} = \infty$. The accuracy of the reconstruction from TV and NN regularization depends on the value of the regularization parameter α , while the accuracy of the reconstruction from NTGV regularization depends on the regularization parameters α and β . For all methods, a range of regularization parameters was considered, and the regularization parameter which gave the largest PSNR was chosen.

The results reported in this work correspond to the reconstructions obtained using these parameter values.

For completeness, NTGV regularization could be turned into a one-parameter regularization technique by heuristically constraining α and β to be functions of each other, as was done in the work of Recic *et al.* [57]. For systems in which no ground truth is known, the independent regularization parameter could then be chosen using any of the techniques described in the work of Mitchell *et al.* [58]. These extensions have not been pursued in the present work but could be the focus of future investigations.

The T_2 maps which would result from the reconstructed T_2 -weighted images are not compared quantitatively, because the step of obtaining the T_2 map commonly involves another regularization step, which introduces some uncertainty because of the need to choose the regularization parameter. However, an illustration of the T_2 map obtained using L_1 regularization is given in Section 4.

4. Results and discussion

The results of the reconstructions of the T_2 -weighted images from the undersampled MRI data using different techniques are now presented. For illustration, only the results corresponding to the experimental data acquired at the lowest sampling percentage, 3.1% of k -space, are shown.

Fig. 3 shows the reconstructions of the T_2 -weighted images using zero-filling, TV regularization, NN regularization and NTGV regularization for a coherent sampling pattern. An example is given for two selected slices (one transverse and one longitudinal) through the 3D sample; data are shown for the 10th echo. These images are also compared with the corresponding images obtained from the fully sampled MRI data. It is observed that the ZF reconstructions are poor and dominated by undersampling artefacts; it is not possible to distinguish between the different tubes present in the sample. The application of TV regularization gives a significant improvement, but the reconstructions have artificial staircasing features, as illustrated in Fig. 3(a), a well-known feature of over-regularization in TV regularization [46]. The boundary between some of the tubes is not very clear, particularly in the transverse slice image. The reconstructions obtained from NN regularization seem slightly worse than the

reconstructions obtained from TV regularization; more noise is observed both within and outside the tubes, although the tubes are more clearly distinguished. NTGV regularization gives improved reconstructions over TV and NN regularization, although not noticeably. The NTGV regularization reconstructions inherit good features from TV and NN regularization: the noise level is reduced (a TV regularization property) and the tubes are clearly distinguished (a NN regularization property).

Fig. 4 shows the reconstructions of the T_2 -weighted images using zero-filling, TV regularization, NN regularization and NTGV regularization for an incoherent sampling pattern. Again, ZF reconstructions are poor and dominated by undersampling artefacts. The reconstructions obtained from TV regularization are similar to the results from TV regularization in Fig. 3, where the sampling pattern was coherent. This is explained by the fact that TV regularization is imposed on each individual 3D T_2 -weighted image independently of the other 3D T_2 -weighted images. Therefore, whether the sampling pattern for the corresponding k -space of the different T_2 -weighted images is the same or different does not make a noticeable difference. The reconstructions obtained from NN regularization show significant improvement both over TV and NN reconstructions obtained using a coherent sampling pattern. This significant improvement in the NN regularization performance is explained by the fact that NN regularization relies on the correlation between the different T_2 -weighted images. Therefore, having different sampling patterns for the corresponding k -space of the different T_2 -weighted images reduces the coherent artefacts that are introduced using a coherent sampling pattern. NTGV regularization gives further improvement in performance over TV and NN regularization. NTGV reconstructions inherit good features from TV and NN regularization, similar to the case of a coherent sampling pattern.

A quantitative comparison using the PSNR metric between the reconstructions obtained using zero-filling, TV regularization, NN regularization and NTGV regularization is presented in Fig. 5. The comparison is made over the different sampling percentages studied: 50%, 25%, 12.5%, 6.3% and 3.1% of k -space. Fig. 5(a) shows the results for a coherent sampling pattern. At all sampling percentages, NTGV regularization outperforms TV regularization, which in turn outperforms NN regularization. All the regularization techniques perform better than zero-filling. These results agree with the qualitative observations in Fig. 3. However, the performance gap between NTGV regularization and TV regularization is negligible, suggesting that when a coherent

sampling pattern is used, there is only a small benefit in using NTGV regularization over the conventional TV regularization. Fig. 5(b) shows the results for an incoherent sampling pattern. The first observation is that NTGV regularization still remains the most accurate reconstruction method. The performance gap between NTGV regularization and the other regularization techniques has increased. In addition, the performance of NTGV regularization for an incoherent sampling pattern is significantly better than for a coherent sampling pattern. These two observations suggest that the full potential of NTGV regularization is only realized when an incoherent sampling pattern is used. This is consistent with the earlier discussion. It is also observed that the performance of NN regularization is significantly improved from the case of a coherent sampling pattern and its performance is better than TV regularization, unlike for the case of a coherent sampling pattern. Further, the performance of TV regularization and zero-filling is observed to be similar to when using a coherent sampling pattern, as expected.

The results presented in this section suggest that using an incoherent sampling pattern and NTGV regularization as the reconstruction technique gives the best reconstructions at all sampling percentages studied, according to the PSNR metric. In practice, there are other factors that one might want to consider when choosing the best reconstruction technique. An important factor is that NTGV regularization is a two-parameter regularization technique, as opposed to TV regularization and NN regularization which are one-parameter regularization techniques. Further, the convergence speed for the numerical solution of the NTGV regularization problem is slower than the convergence speed for the numerical solution of the TV regularization and NN regularization methods; typically 3-5 times more iterations are needed and the time per iteration is approximately double for NTGV regularization, as compared to TV and NN regularization. Both these factors make the processing time for the NTGV regularization method longer than the processing time for TV and NN regularization. This observation is particularly important when the sampling percentage is large. For example, at sampling percentages of 25% and 50% of k -space, no visible difference between the reconstructions obtained from the different techniques was observed, although the PSNR metric reveals some differences. Therefore, at the high sampling percentages of 25% and 50% of k -space, the small gain in image quality from NTGV regularization over TV and

NN regularization may be outweighed by the larger processing time of NTGV regularization.

For completeness, the 3D T_2 maps obtained from the T_2 -weighted images are now considered. Each pixel in the 3D image is assigned a T_2 distribution by using L_1 regularization [43] to convert the decay of the pixel intensity into a T_2 distribution. As this step is not the focus of the paper, only an example is presented; the optimisation of the L_1 regularization technique is not considered. Fig. 6 shows the spatially-resolved T_2 distribution over a line through the 3D image (1D T_2 map), whose location is annotated in Fig. 4(a). The line over which the T_2 mapping is performed runs through the tube filled with fluids D and A, whose bulk T_2 distributions are given in Fig. 1(b). Fig. 6(a) shows the results obtained from the T_2 -weighted images of the fully sampled data. Fig. 6(b) shows the results obtained from the T_2 -weighted images reconstructed from the MRI data acquired at 3.1% sampling of k -space and an incoherent sampling pattern, processed using NTGV regularization. The position of the peaks in the T_2 distributions of fluids A (peak 1) and D (peaks 2 and 3), and the relative intensities of peaks 2 and 3 are summarised in Table 1. It is observed that the 1D T_2 maps obtained from both the fully sampled and undersampled data are in good agreement with the bulk liquid measurements in Fig. 1(b). The positions of peaks 1 and 2, as obtained from Fig. 6(a) and 6(b) are $< 15\%$ different from the results in Fig. 1(b). The position of peak 3 is less well predicted from the 3D T_2 maps of both fully sampled and undersampled data; this is mainly due to the low intensity of this peak as compared to peak 2. For fluid D, the fraction of the total intensity represented by peak 2, obtained from Figs. 1(b), 6(a) and 6(b) are in reasonable agreement; respectively 0.67, 0.82 ± 0.07 and 0.73 ± 0.05 . The quoted uncertainty for the spatially-resolved intensity data from Figs. 6(a) and 6(b) refers to the spatial variation of the intensity fraction represented by peak 2. Other sources of uncertainty for the intensity fraction data from Figs. 1(b), 6(a) and 6(b), such as from L_1 regularization, are not reported and could explain why the reported intensity fraction intervals from the different methods do not fully overlap. The fact that the two peaks in the T_2 distribution of fluid D can be distinguished and quantified to a reasonable degree even from highly undersampled data is an achievement of the proposed sampling scheme and processing method. Indeed, it is shown in a related study [59] that bi-exponential decays where the population of one of the components is small are challenging to resolve even from 1D NMR experiments.

5. Conclusions

This work describes an experimental implementation of an MESE pulse sequence for the acquisition of undersampled MRI data, with the aim of obtaining a 3D T_2 map. Two classes of sampling patterns were compared: a conventional coherent sampling pattern where the same set of lines in k -space is sampled for all equally-spaced echoes in the echo train, and a proposed incoherent sampling pattern where a different set of k -space lines is sampled for each. The conventional reconstruction technique of TV regularization was compared to the more recent techniques of NN and NTGV regularization. It was observed that the use of an incoherent sampling pattern leads to a better reconstruction quality than the use of a coherent sampling pattern. NTGV regularization outperformed TV regularization and NN regularization at all sampling percentages studied, although the difference was small at sampling percentages $>25\%$. The full potential of NTGV regularization is particularly realized when an incoherent sampling pattern is used. Using an incoherent sampling scheme and NTGV regularization as the reconstruction technique, quantitative results were obtained even at a sampling percentage of 3.1% of k -space, corresponding to a 32-fold decrease in the acquisition time.

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Appendix

This Appendix provides pseudocodes for the numerical reconstruction of 3D T_2 -weighted images from undersampled MRI data obtained using an MESE pulse sequence. Pseudocodes for three different type of reconstructions are presented: TV regularization, NN regularization and NTGV regularization.

a) TV regularization

The minimization problem in Eq. (3) can be written as:

$$\underline{u} = \arg \min_{\underline{u}} \max_{\underline{z}} \left(\frac{1}{2} \left\| \underline{S} \underline{F} \underline{u} - \underline{y} \right\|_2^2 + \underline{z}^T \underline{R} \underline{u} - h(\underline{z}) \right), \quad (\text{A1})$$

where \underline{z} is a $3n^3p \times 1$ vector, called a dual variable, and $h(\underline{z})$ is an indicator function [60] defined as:

$$h(\underline{z}) = \begin{cases} 0 & \|\underline{z}\|_{2,\infty} \leq \alpha \\ +\infty & \|\underline{z}\|_{2,\infty} > \alpha \end{cases}. \quad (\text{A2})$$

$\|\underline{z}\|_{2,\infty}$ is defined as in the work of Chambolle and Pock [61]. Eq. (A1) is a primal-dual optimization problem which can be numerically solved by a Primal-Dual Hybrid Gradient Method (PDHGM) [56]. A pseudocode describing the steps in the algorithm follows. In the pseudocode: `reshape(\underline{A} , [n_1, n_2, \dots, n_j])` reshapes the $n_1 n_2 \dots n_j \times 1$ vector \underline{A} into a $n_1 \times n_2 \times \dots \times n_j$ matrix; `sum(\underline{A} , i)` sums the elements of matrix \underline{A} along the i -th dimension; and `repmat(\underline{A} , k , i)` stacks k copies of \underline{A} in the i -th dimension.

Step 1. Choose the algorithm parameters τ, σ and the regularization parameters α .

Step 2. Set the convergence tolerance, TOL .

Step 3. Initialize $\underline{u}^{(0)} = \underline{0}$, $\underline{z}^{(0)} \neq \underline{0}$, $\underline{u}_1^{(0)} = \underline{u}^{(0)}$.

Step 4. Initialize count number, $k = 1$, and convergence tracker, $\epsilon^{(0)} = 1$.

Step 5. **while** $\epsilon^{(k-1)} > TOL$ **do**

$$\text{a. } \underline{z}_1 \leftarrow \underline{z}^{(k-1)} + \sigma R \underline{u}_1^{(k-1)}$$

$$\text{b. } \underline{z}_2 \leftarrow \sqrt{\text{sum} \left(\left| \text{reshape} \left(\left(\underline{z}_1 \right)^2, [n^3 p, 3] \right) \right|, 2 \right)}$$

The square root operation is element-wise.

$$\text{c. } \underline{z}^{(k)} \leftarrow \frac{\underline{z}_2}{\max(1, \text{repmat}(\underline{z}_2, 3, 1)/\alpha)}$$

All operations in this step are element-wise.

$$\text{d. } \underline{u}_2 \leftarrow \underline{u}^{(k-1)} - \tau \underline{R}^T \underline{z}^{(k)}$$

$$\text{e. } \underline{u}^{(k)} \leftarrow \underline{F}^{-1} \left(\frac{\underline{F} \underline{u}_2 + \tau \underline{S}^T \underline{y}}{1 + \tau \text{diag}(\underline{S}^T \underline{S})} \right)$$

The division operation is performed element-wise.

$$\text{f. } \underline{u}_1^{(k)} \leftarrow 2\underline{u}^{(k)} - \underline{u}^{(k-1)}$$

$$\text{g. } \epsilon^{(k)} \leftarrow \frac{\|\underline{u}^{(k)} - \underline{u}^{(k-1)}\|_2}{\|\underline{u}^{(k-1)}\|_2}$$

$$\text{h. } k \leftarrow k + 1$$

end while

The condition for the algorithm to converge is $\tau \sigma \leq 1/\|\underline{R}\|^2$. The choice of $\tau = \sigma = 1/\|\underline{R}\|$ was made in this work, where $\|\underline{R}\|^2 \approx 8$. The number of iterations required to arrive at a reasonable convergence was approximately 300. The time in which this convergence was achieved for a $64 \times 64 \times 64 \times 64$ dataset with a 2.0 GHz Intel® Core™ i5-4590T CPU and 16.4 GB RAM, was approximately 6 min.

b) NN regularization

The minimization problem in Eq. (4) can be written as:

$$\underline{u} = \arg \min_{\underline{u}} \max_{\underline{V}} \left(\frac{1}{2} \|\underline{S} \underline{F} \underline{u} - \underline{y}\|_2^2 + \text{trace}(\underline{V}^T \underline{\hat{U}}) - h(\underline{V}) \right), \quad (\text{A3})$$

where \underline{V} is a $n^3 \times p$ matrix, called a dual variable, and $h(\underline{V})$ is an indicator function defined as:

$$h(\underline{V}) = \begin{cases} 0 & \|\underline{V}\|_{S^\infty} \leq \alpha \\ +\infty & \|\underline{V}\|_{S^\infty} > \alpha \end{cases}. \quad (\text{A4})$$

$\|\underline{V}\|_{S^\infty}$ is the Schatten infinity norm, defined in the work of Chambolle and Pock [61]. Eq. (A3) is a primal-dual optimization problem which can be numerically solved by the PDHGM algorithm. A pseudocode describing the steps in the algorithm follows. In the pseudocode: $[\underline{A}_1, \underline{A}_2, \underline{A}_3] = \text{svd}(\underline{A})$, computes the singular value decomposition of \underline{A} , such that $\underline{A} = \underline{A}_1 \underline{A}_2 \underline{A}_3^T$, where \underline{A}_1 and \underline{A}_3 are orthogonal matrices and \underline{A}_2 is a diagonal matrix containing the sorted singular values of \underline{A} .

Step 1. Choose the algorithm parameters τ, σ and the regularization parameters, α .

Step 2. Set the convergence tolerance, TOL .

Step 3. Initialize $\hat{\underline{U}}^{(0)} = \underline{0}$, $\underline{V}^{(0)} \neq \underline{0}$, $\underline{U}_1^{(0)} = \hat{\underline{U}}^{(0)}$.

Step 4. Initialize count number, $k = 1$, and convergence tracker, $\epsilon^{(0)} = 1$.

Step 5. **while** $\epsilon^{(k-1)} > TOL$ **do**

a. $\underline{V}_1 \leftarrow \underline{V}^{(k-1)} + \sigma \underline{U}_1^{(k-1)}$

b. $[\underline{A}_1, \underline{A}_2, \underline{A}_3] \leftarrow \text{svd}(\underline{V}_1)$

c. $\underline{A}_2 \leftarrow \min(\alpha, \underline{A}_2)$

The operation is performed element-wise.

d. $\underline{V}^{(k)} \leftarrow \underline{A}_1 \underline{A}_2 \underline{A}_3^T$

e. $\underline{U}_2 \leftarrow \hat{\underline{U}}^{(k-1)} - \tau \underline{V}^{(k)}$

f. $\hat{\underline{U}}^{(k)} \leftarrow \text{reshape}\left(\underline{F}^{-1}\left(\frac{\underline{F} \text{ reshape}(\underline{U}_2, n^3 p, 1) + \tau \underline{S}^T \underline{y}}{1 + \tau \text{ diag}(\underline{S}^T \underline{S})}\right), [n^3, p]\right)$

The division operation is performed element-wise.

g. $\underline{U}_1^{(k)} \leftarrow 2\hat{\underline{U}}^{(k)} - \hat{\underline{U}}^{(k-1)}$

h. $\epsilon^{(k)} \leftarrow \frac{\|\underline{u}^{(k)} - \underline{u}^{(k-1)}\|_2}{\|\underline{u}^{(k-1)}\|_2}$

i. $k \leftarrow k + 1$

end while

The condition for the algorithm to converge is $\tau \sigma \leq 1$. The choice of $\tau = \sigma = 1$ was made in this work. Note that $\hat{\underline{U}}$ and \underline{u} refer to the same variable, but shaped in different matrix dimensions, as discussed in Section 3. The number of iterations required to arrive at a reasonable convergence was approximately 200. The time in which this convergence was achieved for a $64 \times 64 \times 64 \times 64$ dataset with a 2.0 GHz Intel® Core™ i5-4590T CPU and 16.4 GB RAM, was approximately 4 min.

c) NTGV regularization

The minimization problem in Eq. (5) can be written as:

$$\underline{u} = \arg \min_{\underline{u}, \underline{\hat{w}}} \max_{\underline{V}, \underline{z}} \left(\frac{1}{2} \left\| \underline{S} \underline{F} \underline{u} - \underline{y} \right\|_2^2 + \text{trace} \left(\underline{V}^T (\underline{\hat{U}} - \underline{\hat{W}}) \right) - h_1(\underline{V}) + \underline{z}^T \underline{R} \underline{w} - h_2(\underline{z}) \right), \quad (\text{A5})$$

where \underline{V} is a $n^3 \times p$ matrix and \underline{z} is a $3n^3p \times 1$ vector, called dual variables. $h_1(\underline{V})$ and $h_2(\underline{z})$ are indicator functions defined as:

$$h_1(\underline{V}) = \begin{cases} 0 & \|\underline{V}\|_{S^\infty} \leq \alpha \\ +\infty & \|\underline{V}\|_{S^\infty} > \alpha \end{cases}, \quad (\text{A6a})$$

$$h_2(\underline{z}) = \begin{cases} 0 & \|\underline{z}\|_{2,\infty} \leq \beta \\ +\infty & \|\underline{z}\|_{2,\infty} > \beta \end{cases}. \quad (\text{A6b})$$

Eq. (A5) is a primal-dual optimization problem which can be numerically solved by the PDHGM algorithm. A pseudocode describing the steps in the algorithm follows.

Step 1. Choose the algorithm parameters τ, σ and the regularization parameters α, β .

Step 2. Set the convergence tolerance, TOL .

Step 3. Initialize $\underline{\hat{U}}^{(0)} = \underline{0}, \underline{\hat{W}}^{(0)} = \underline{0}, \underline{V}^{(0)} \neq \underline{0}, \underline{U}_1^{(0)} = \underline{\hat{U}}^{(0)}, \underline{W}_1^{(0)} = \underline{\hat{W}}^{(0)}, \underline{z}^{(0)} \neq \underline{0}$.

Step 4. Initialize count number, $k = 1$, and convergence tracker, $\epsilon^{(0)} = 1$.

Step 5. **while** $\epsilon^{(k-1)} > TOL$ **do**

$$\text{a. } \underline{V}_1 \leftarrow \underline{V}^{(k-1)} + \sigma \left(\underline{U}_1^{(k-1)} - \underline{W}_1^{(k-1)} \right)$$

$$\text{b. } [\underline{A}_1, \underline{A}_2, \underline{A}_3] \leftarrow \text{svd}(\underline{V}_1)$$

$$\text{c. } \underline{A}_2 \leftarrow \min(\alpha, \underline{A}_2)$$

The operation is performed element-wise.

$$\text{d. } \underline{V}^{(k)} \leftarrow \underline{A}_1 \underline{A}_2 \underline{A}_3^T$$

$$\text{e. } \underline{U}_2 \leftarrow \underline{\hat{U}}^{(k-1)} - \tau \underline{V}^{(k)}$$

$$\text{f. } \underline{\hat{U}}^{(k)} \leftarrow \text{reshape} \left(\underline{F}^{-1} \left(\frac{\underline{F} \text{reshape}(\underline{U}_2, n^3p, 1) + \tau \underline{S}^T \underline{y}}{1 + \tau \text{diag}(\underline{S}^T \underline{S})} \right), [n^3, p] \right)$$

The division operation is performed element-wise.

$$\text{g. } \underline{z}_1 = \underline{z}^{(k-1)} + \sigma \underline{R} \text{reshape}(\underline{W}_1^{(k-1)}, n^3p, 1)$$

$$\text{h. } \underline{z}_2 \leftarrow \sqrt{\text{sum} \left(\left| \text{reshape} \left((\underline{z}_1)^2, [n^3p, 3] \right) \right|, 2 \right)}$$

The square root operation is element-wise.

$$\text{i. } \underline{z}^{(k)} \leftarrow \frac{\underline{z}_2}{\max(1, \text{repmat}(\underline{z}_2, 3, 1)/\beta)}$$

All operations in this step are element-wise.

$$\text{j. } \underline{\hat{W}}^{(k)} \leftarrow \underline{\hat{W}}^{(k-1)} + \tau \left(\underline{V}^{(k)} - \text{reshape}(\underline{R}^T \underline{z}^{(k)}, [n^3, p]) \right)$$

$$\text{k. } \underline{U}_1^{(k)} \leftarrow 2\underline{\hat{U}}^{(k)} - \underline{\hat{U}}^{(k-1)}$$

$$\text{l. } \underline{W}_1^{(k)} \leftarrow 2\underline{\hat{W}}^{(k)} - \underline{\hat{W}}^{(k-1)}$$

$$\text{m. } \epsilon^{(k)} \leftarrow \frac{\|\underline{u}^{(k)} - \underline{u}^{(k-1)}\|_2}{\|\underline{u}^{(k-1)}\|_2}$$

$$\text{n. } k \leftarrow k + 1$$

end while

The condition for the algorithm to converge is $\tau \sigma \leq 1/12$. The choice of $\tau = \sigma \approx 0.28$ was made in this work. Note that $\underline{\hat{U}}$ and \underline{u} refer to the same variable, but shaped in different matrix dimensions, as discussed in section 3. Similarly, $\underline{\hat{W}}$ and \underline{w} refer to the same variable, but shaped in different matrix dimensions. The number of iterations required to arrive at a reasonable convergence was approximately 1000. The time in which this convergence was achieved for a $64 \times 64 \times 64 \times 64$ dataset with a 2.0 GHz Intel® Core™ i5-4590T CPU and 16.4 GB RAM, was approximately 1 h.

1.

2.

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Figure captions

Fig. 1. (a) Schematic arrangement of the tubes used in the experiments (not to scale). Each tube is filled in the bottom half with a gadolinium chloride solution (A, B or C) and on the top half with PDMS oil (D, E or F). (b) T_2 distributions of each fluid used in the experiment, A-F, obtained from bulk fluid measurements using a single shot CPMG pulse sequence.

Fig. 2. The sampling pattern used for the first two echoes and for the two dimensions of k -space which can be randomly undersampled; the patterns are shown for 3.1% sampling of k -space. Patterns are shown for (a) a coherent sampling pattern and (b) an incoherent sampling pattern.

Fig. 3. Comparison of the T_2 -weighted images obtained from a fully sampled dataset with the reconstructed T_2 -weighted images obtained using ZF, TV regularization, NN regularization and NTGV regularization for a coherent sampling pattern. The data are shown for a sampling percentage of 3.1% of k -space. (a) An example of a transverse T_2 -weighted image through the tubes at a position shown in (b) and echo number 10. (b) An example of a longitudinal T_2 -weighted image through the tubes at a position shown in (a) and echo number 10. The highlighted region of the TV reconstruction in (a) illustrates the artificial staircasing, a common feature of over-regularization in the application of TV regularization.

Fig. 4. Comparison of the T_2 -weighted images obtained from a fully sampled dataset with the reconstructed T_2 -weighted images obtained using ZF, TV regularization, NN regularization and NTGV regularization for an incoherent sampling pattern. The data are shown for a sampling percentage of 3.1% of k -space. (a) An example of a transverse T_2 -weighted image through the tubes at a position shown in (b) and echo number 10. (b) An example of a longitudinal T_2 -weighted image through the tubes at a position shown in (a) and echo number 10. The ‘+’ marker in the fully sampled image of (a) denotes the projection of the line over which the T_2 mapping shown in Fig. 6 is taken. The distance ‘ z ’ in (b) corresponds to the distance ‘ z ’ used in Fig. 6.

Fig. 5. Comparison of the different techniques: ZF, TV regularization, NN regularization and NTGV regularization in reconstructing the T_2 -weighted images from undersampled MRI data at different sampling percentages. Data are shown for (a) a coherent and (b) an

incoherent sampling pattern. The PSNR metric is defined in Eq. (6). The lines are included to guide the eye.

Fig. 6. 1D T_2 maps over the line denoted in Fig. 4(a). The 1D T_2 maps were obtained from (a) the fully sampled dataset and, (b) the data acquired at 3.1% sampling of k -space data using an incoherent sampling pattern and processed using NTGV regularization. The line over which the mapping is performed runs through fluids D and A. The distance z is defined in Fig. 4(b).

Tables

Table 1: Estimation of the position of the peaks in the T_2 distribution of fluids A (peak 1) and D (peaks 2 and 3), and the fraction of total intensity of fluid D represented by peak 2, determined using three different measurements. The bulk measurement is taken from Fig. 1(b). The measurement from the fully sampled dataset is taken from Fig. 6(a). The measurement from the undersampled dataset is taken from Fig. 6(b). The peaks are annotated in Fig. 6(a). The uncertainty shown corresponds to the spatial variation of the properties, as observed from Fig. 6.

	T_2 / ms			intensity fraction peak 2 / (peak 2+peak 3)
	peak 1	peak 2	peak 3	
bulk measurement	87	140	380	0.67
fully sampled dataset	88 ± 3	160 ± 10	600 ± 160	0.82 ± 0.07
undersampled dataset	98 ± 8	130 ± 10	540 ± 90	0.73 ± 0.05











